Introduction to Machine Learning

Feature Generation

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February 25, 2019

Outline

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What do we want?

What

Given a set of measurements, the goal is to discover compact and informative representations of the obtained data.

Our Approach

We want to "squeeze" in a relatively small number of features, leading to a reduction of the necessary feature space dimension.

Properties

Thus removing information redundancies - Usually produced and the measurement.

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What Methods we will see?

Fisher Linear Discriminant

1. Squeezing to the maximum.
2. From Many to One Dimension

Principal Component Analysis

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However, Please review

Singular Value Decomposition

1. Decompose a $m \times n$ data matrix A into $A = USV^T$, U and V orthonormal matrices and S contains the eigenvalues.
2. You can read more of it on “Singular Value Decomposition Tutorial” at the paper section.

Outline

Rotation

Projecting

Projecting well-separated samples onto an arbitrary line usually produces a confused mixture of samples from all of the classes and thus produces poor recognition performance.

Something Notable

However, moving and rotating the line around might result in an orientation for which the projected samples are well separated.

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It is a discriminant analysis seeking directions that are efficient for discriminating binary classification problem.

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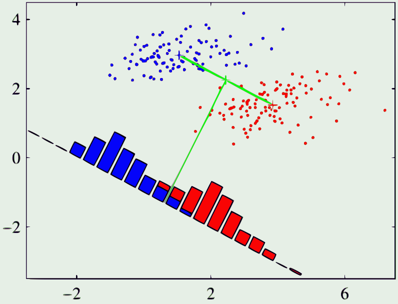
Example

Example - From Left to Right the Improvement



This is actually comming from...

Classifier as

A machine for dimensionality reduction.

Initial Setup

We have:

- N d-dimensional samples $x_1, x_2, ..., x_N$
- N_i is the number of samples in class C_i for i=1,2.

Then, we ask for the projection of each x_i into the line by means of

$$y_i = w^T x_i \tag{1}$$

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Use the mean of each Class

Then

Select $\boldsymbol{w}$ such that class separation is maximized

We then define the mean sample for ecah class

1. $C_1 \Rightarrow \boldsymbol{m}_1 = \frac{1}{N_1}\sum_{i=1}^{N_1} \boldsymbol{x}_i$
2. $C_2 \Rightarrow \boldsymbol{m}_2 = \frac{1}{N_2}\sum_{i=1}^{N_2} \boldsymbol{x}_i$

Ok!!! This is giving us a measure of distance

Thus, we want to maximize the distance the projected means:

$$m_1 - m_2 = \boldsymbol{w}^T (\boldsymbol{m}_1 - \boldsymbol{m}_2) \tag{2}$$

where $m_k = \boldsymbol{w}^T \boldsymbol{m}_k$ for $k = 1, 2$.

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After all

We do not care about the magnitude of w.

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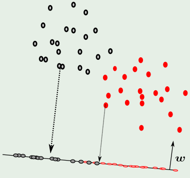

Outline

Fixing the Problem

To obtain good separation of the projected data

The difference between the means should be large relative to some measure of the standard deviations for each class.

We define a SCATTER measure (Based in the Sample Variance)

$$s_k^2 = \sum_{x_i \in C_k} \left(w^T x_i - m_k \right)^2 = \sum_{y_i = w^T x_i \in C_k} \left(y_i - m_k \right)^2 \tag{3}$$

We define then within-class variance for the whole data

$$s_1^2 + s_2^2 \tag{4}$$

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Finally, a Cost Function

The between-class variance

$$(m_1 - m_2)^2 \tag{5}$$

The Fisher criterion

$$\frac{\text{between-class variance}}{\text{within-class variance}} \tag{6}$$

Finally

$$J(w) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2} \tag{7}$$

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An approximation to the $\boldsymbol{w}$

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- Use a threshold $y_0 \Rightarrow x \in C_1$ iff $y(x) \geq y_0$ or $x \in C_2$ iff $y(x) < y_0$
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Please

Your Reading Material, it is about the Multiclass

4.1.6 Fisher's discriminant for multiple classes AT “Pattern Recognition” by Bishop

Outline

Also Known as Karhunen-Loeve Transform

Setup

- Consider a data set of observations $\{\boldsymbol{x}_n\}$ with $n = 1, 2, ..., N$ and $\boldsymbol{x_n} \in R^d$.

Goal

Project data onto space with dimensionality $m < d$ (We assume m is given)

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Dimensional Variance

Remember the Sample Variance Sample

$$VAR(X) = \frac{\sum_{i=1}^{N} (x_i - \overline{x})(x_i - \overline{x})}{N-1} \tag{9}$$

You can do the same in the case of two variables X and Y

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Given the data

$$\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_N \tag{11}$$

where $\boldsymbol{x}_i$ is a column vector

Construct the sample mean

$$\overline{\boldsymbol{x}} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}_i \tag{12}$$

Build new data

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The Covariance Matrix

$$S = \frac{1}{N-1}\sum_{i=1}^{N}\left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)^T \tag{14}$$

Properties

1. The ijth value of S is equivalent to σ_{ij}^2.
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3. What else? Look at a plane Center and Rotating!!!

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Using S to Project Data

As in Fisher

We want to project the data to a line...

For this we use a u_1

with $u_1^T u_1 = 1$

Question

What is the Sample Variance of the Projected Data

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Thus we have

Variance of the projected data

$$\frac{1}{N-1}\sum_{i=1}^{N}\left[\boldsymbol{u}_1\boldsymbol{x}_i-\boldsymbol{u}_1\overline{\boldsymbol{x}}\right]=\boldsymbol{u}_1^T S\boldsymbol{u}_1 \tag{15}$$

Use Lagrange Multipliers to Maximize

$$\boldsymbol{u}_1^T S\boldsymbol{u}_1+\lambda_1\left(1-\boldsymbol{u}_1^T\boldsymbol{u}_1\right) \tag{16}$$

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$\boldsymbol{u}_1$ is an eigenvector of S.

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What about the second eigenvector $\boldsymbol{u}_2$

We have the following optimization problem

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Lagrangian

$$L\left(\boldsymbol{u}_2, \lambda_1, \lambda_2\right) = \boldsymbol{u}_2^T S \boldsymbol{u}_2 - \lambda_2 \left(\boldsymbol{u}_2^T \boldsymbol{u}_2 - 1\right) - \lambda_1 \left(\boldsymbol{u}_2^T \boldsymbol{u}_1 - 0\right)$$

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Thus

Variance will be the maximum when

$$\boldsymbol{u}_1^T S \boldsymbol{u}_1 = \lambda_1 \tag{19}$$

is set to the largest eigenvalue. Also know as the First Principal Component

By Induction

It is possible for M-dimensional space to define M eigenvectors $\boldsymbol{u}_1, \boldsymbol{u}_2, ..., \boldsymbol{u}_M$ of the data covariance S corresponding to $\lambda_1, \lambda_2, ..., \lambda_M$ that maximize the variance of the projected data.

Computational Cost

1. Full eigenvector decomposition $O\left(d^3\right)$
2. Power Method $O\left(Md^2\right)$ "Golub and Van Loan, 1996)"
3. Use the Expectation Maximization Algorithm

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$$S = U\Sigma U^T$$

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- Eigenvalues in Σ and eigenvectors in the columns of U.

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Then

Project samples $\boldsymbol{x}_i$ into subspaces dim$=k$

$$z_i = U_K^T \boldsymbol{x}_i$$

- With U_k is a matrix with k columns

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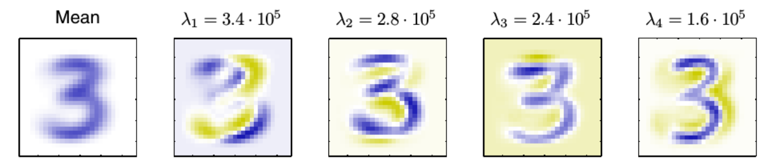

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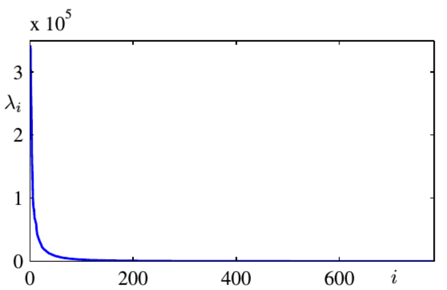

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